EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	119	(548/401).CCLS.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	OR	OFF	2007/12/09 19:05
L2	262	(548/405).CCLS.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	OR	OFF	2007/12/09 19:06
L3	3	l1 and l2	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	OR	ON	2007/12/09 19:06

EAST Search History

L4	1	l1 and oxazaborolidine	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	OR	ON	2007/12/09 19:06
L5	7	l2 and oxazaborolidine	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	OR	ON	2007/12/09 19:06

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```
=> s oxazaborolidine
           558 OXAZABOROLIDINE
           215 OXAZABOROLIDINES
L1         605 OXAZABOROLIDINE
                 (OXAZABOROLIDINE OR OXAZABOROLIDINES)

=> s l1 and complexes
        759694 COMPLEXES
             4 COMPLEXESES
        759695 COMPLEXES
                 (COMPLEXES OR COMPLEXESES)
L2          52 L1 AND COMPLEXES

=> s l2 and chiral
        119944 CHIRAL
            17 CHIRALS
        119948 CHIRAL
                 (CHIRAL OR CHIRALS)
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L3          32 L2 AND CHIRAL

=> s l3 and in(l)situ
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          6731 INS
          6731 IN
                 (IN OR INS)
        276067 SITU
           272 SITUS
        276324 SITU
                 (SITU OR SITUS)
           131 IN(L)SITU
L4           0 L3 AND IN(L)SITU

=> d l3 ibib abs hitstr tot
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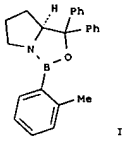
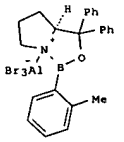
L3 ANSWER 1 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:76720 CAPLUS
DOCUMENT NUMBER: 146:337266
TITLE: Chiral Oxazaborolidine-Aluminum Bromide Complexes Are Unusually Powerful and Effective Catalysts for Enantioselective Diels-Alder Reactions
AUTHOR(S): Liu, Duan; Canales, Eda; Corey, E. J.
CORPORATE SOURCE: Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA
SOURCE: Journal of the American Chemical Society (2007), 129(6), 1498-1499
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:337266
GI



I



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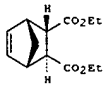


III

AB Treatment of the chiral oxazaborolidine I with AlBr3 generates the 1:1 complex II, which is an even more potent Lewis acid catalyst than protonated I for enantioselective Diels-Alder reactions. Only 4 mol % of catalyst II is required to achieve yields and enantiomeric purities of 90% over a broad range of achiral dienes and dienophiles. The ligand from which II is derived can be recovered easily and with high efficiency. The method is illustrated by 22 examples. E.g., Diels-Alder reaction of cyclopentadiene and di-Et fumarate, catalyzed by II, gave

L3 ANSWER 1 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
product III.
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:39912 CAPLUS
DOCUMENT NUMBER: 147:501894
TITLE: Asymmetric reduction of prochiral ketones
AUTHOR(S): Zhou, Zhongqiang
CORPORATE SOURCE: College of Chemistry and Materials Science, SCUFN, Wuhan, 430074, Peop. Rep. China
SOURCE: Zhongnan Minzu Daxue Xuebao, Ziran Kexueban (2006), 25(3), 27-32
CODEN: ZMDXA3; ISSN: 1672-4321
PUBLISHER: Zhongnan Minzu Daxue Xuebao Bianjibu
DOCUMENT TYPE: Journal; General Review
LANGUAGE: Chinese
AB A review. In this review, the asym. reduction of prochiral ketones and its recent advances have been described, including application of chiral oxazaborolidine catalysts, reduction by chirally modified lithium aluminum hydride reagents, application of chirally modified sodium borohydride or potassium borohydride, application of chiral phosphoramide catalysts, transfer hydrogenation of prochiral ketones catalyzed by chiral metal complexes, asym. reduction of prochiral ketones by phase-transfer catalysis, enantioselective reduction of ketones with enzymes.

L3 ANSWER 3 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:23509 CAPLUS
DOCUMENT NUMBER: 146:296026
TITLE: The Mg-Oppenauer oxidation as a mild method for the synthesis of aryl and metallocenyl ketones
AUTHOR(S): Kloetzing, Ralf J.; Krasovskiy, Arkady; Knochel, Paul
CORPORATE SOURCE: Dep. Chem. Biochem., Ludwig-Maximilians-Univ., Munich, 81377, Germany
SOURCE: Chemistry--A European Journal (2006), 13(1), 215-227
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:296026
AB Mg alkoxides undergo a hydride-transfer oxidation with benzaldehyde as the oxidant. This Mg variant of the Oppenauer oxidation was used for the synthesis of polyfunctional biaryl ketones. LiCl was found to promote this reaction by enhancing the solubility of Mg alkoxides. Twelve functionalized unsym. diaryl ketones were prepared from the corresponding Mg alkoxides in 85% to 98% yields. E.g., 2-bromobenzophenone was obtained in 91% yield by reaction of phenylmagnesium chloride with 2-bromobenzaldehyde in the presence of LiCl, followed by oxidation with benzaldehyde. Neither electron-accepting nor -donating substituents appear to influence the reaction course. Although one ortho-substituent does not retard the reaction, the presence of two ortho-substituents inhibited the Mg-Oppenauer reaction completely due to the high steric hindrance. This mild oxidation method was especially useful for preparing ketones bearing a metallocenyl unit as well as various new ferrocenyl ketones and tricarbonylchromium complexes. Addition of PhMgCl·LiCl to cymantrene aldehyde and oxidation with benzaldehyde afforded benzoylcymantrene in 80% yield. Various aromatic Grignard reagents were also readily added to tricarbonylchromium benzaldehyde within 10 min at -20°. Oxidation with benzaldehyde within 12 h at room temperature gave the ketones. E.g., addition of 4-Me2NC6H4MgBr·LiCl (from 4-Me2NC6H4Br, Mg and LiCl) to tricarbonylchromium benzaldehyde and oxidation with benzaldehyde gave 4-N,N-dimethylaminobenzoyltricarbonylchromium in 92% yield. With nonfunctionalized or electron-rich ketones, 65% to 92% yields were obtained. With halogenated arylmagnesium reagents, 28% to 59% yields were observed This last class of ketones was reduced with the CBS catalyst (CBS = Corey-Bakshi-Shibata, di-Ph oxazaborolidine) and decomplexed with iodine to give in 89% to quant. yield chiral benzhydrol complexes with high enantioselectivity enabling an asym. synthesis of electron-rich or -poor benzhydryl alcs. (up to 94% ee). E.g., reduction of 4-methoxybenzoyltricarbonylchromium benzene with borane-dimethyl sulfide complex, followed by decomplexation with iodine gave (R)-(4-methoxyphenyl)phenylmethanol in 90% yield and 93% ee.
REFERENCE COUNT: 123 THERE ARE 123 CITED REFERENCES AVAILABLE FOR

L3 ANSWER 3 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L3 ANSWER 4 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:645325 CAPLUS
DOCUMENT NUMBER: 146:251249
TITLE: Asymmetric reduction of prochiral ketones
AUTHOR(S): Zhou, Zhongqiang
CORPORATE SOURCE: College of Chemistry and Materials Science, SCUFN, Wuhan, 430074, Peop. Rep. China
SOURCE: Zhongnan Minzu Daxue Xuebao, Ziran Kexueban (2006), 25(1), 22-27, 31
CODEN: ZMDXA3; ISSN: 1672-4321
PUBLISHER: Zhongnan Minzu Daxue Xuebao Bianjibu
DOCUMENT TYPE: Journal; General Review
LANGUAGE: Chinese
AB In this review, asym. reduction of prochiral ketones and its recent advances have been described, including application of chiral oxazaborolidine catalysts, reduction by chirally modified lithium aluminum hydride reagents, application of chirally modified sodium borohydride or potassium borohydride, application of chiral phosphoramide catalysts, transfer hydrogenation of prochiral ketones catalyzed by chiral metal complexes, asym. reduction of prochiral ketones by phase-transfer catalysis, enantioselective reduction of ketones with enzyme. A review.

L3 ANSWER 5 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:740583 CAPLUS
TITLE: Enantioselective cyclopropyl ketone-based halo aldol reactions
AUTHOR(S): Li, Guigen; Timmons, Cody
CORPORATE SOURCE: Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX, 79409, USA
SOURCE: Abstracts of Papers, 230th ACS National Meeting, Washington, DC, United States, Aug. 28-Sept. 1, 2005 (2005), ORGN-535. American Chemical Society: Washington, D. C.
CODEN: 69HFCL
DOCUMENT TYPE: Conference; Meeting Abstract; (computer optical disk)
LANGUAGE: English
AB Novel asym. halo aldol-type reactions have been developed using enolates derived from cyclopropyl ketones. The enolate is formed by reacting cyclopropyl ketones with trimethylsilyl iodide. Subsequent addition to aldehydes is promoted by chiral oxazaborolidine complexes, which are easily generated in situ by treating a protected amino acid with borane. A variety of amino acids and protecting groups were screened, and N-heptafluorobutyryl-phenylalanine was found to be optimal for controlling enantioselectivity. Calcns. have been performed to characterize the nature of the enantio-induction. In a similar manner, sulfonyl-protected imines have given promising results when chiral aluminum complexes are used.

L3 ANSWER 6 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:325360 CAPLUS
DOCUMENT NUMBER: 142:392277
TITLE: In situ preparation of chiral compounds derived from oxazaborolidine-borane complexes and their use as catalysts in asymmetric reductions of ketones and ether oximes
INVENTOR(S): Burgos, Alain; Bertrand, Blandine; Frein, Stephane; Pluvie, Jean Francois; Roussiasse, Sonia
PATENT ASSIGNEE(S): PPG-Sipsy, Fr.
SOURCE: Fr. Demande, 30 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

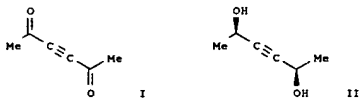
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2860794	A1	20050415	FR 2003-11838	20031009
FR 2860794	B1	20060203		
FR 2860795	A1	20050415	FR 2004-10701	20041011
FR 2860795	B1	20060407		
WO 2005035540	A2	20050421	WO 2004-FR2573	20041011
WO 2005035540	A3	20050609		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1673375	A2	20060628	EP 2004-817157	20041011
EP 1673375	B1	20070801		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1867571	A	20061122	CN 2004-80029618	20041011
JP 2007508280	T	20070405	JP 2006-530431	20041011
AT 368672	T	20070815	AT 2004-817157	20041011
KR 2007026314	A	20070308	KR 2006-706544	20060405
US 2007055068	A1	20070308	US 2006-574871	20060406
PRIORITY APPLN. INFO.:			FR 2003-11838 A	20031009
			WO 2004-FR2573 W	20041011

OTHER SOURCE(S): MARPAT 142:392277
AB The invention is related to the in situ preparation of chiral compds. derived from oxazaborolidine-borane complexes by reacting a metal borohydride with a Lewis base, and an ester of an inorg. acid, followed by addition of an optically active amino-alc. and to their use in the preparation of chiral alcs. and ketones by asym. reduction of prochiral ketones and ether oximes. The method eliminates the use of I2 in the preparation of the oxazaborolidine-borane complex. Thus, NaBH4 in THF was mixed with PhNEt2, the mixture cooled to 5°, Me2SO4 added and the mixture stirred at 20° for 1 h, and finally mixed with

L3 ANSWER 6 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(R)-diphenylprolinol at 20° for 1 h. A soln. of
3-chloro-1-(2-thienyl)propanone in THF was added to the above preheated
mixt. over a period of 1.5 h, followed by hydrolysis for 1 h at 20°
to give the corresponding alc. in high chem. purity.
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L3 ANSWER 7 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:1053291 CAPLUS
DOCUMENT NUMBER: 143:305917
TITLE: Synthesis of chiral amino alcohols by enantioselective borane reduction
AUTHOR(S): Shen, Zong-xuan; Li, Yong-hua; Qin, Hong-bing; Zhang, Ya-wen
CORPORATE SOURCE: Key Lab of Organic Synthesis of Jiangsu Province, College of Chemistry and Chemical Engineering, Suzhou University, Suzhou, Jiangsu, 215006, Peop. Rep. China
SOURCE: Huaxue Yanjiu (2004), 15(3), 23-26, 49
CODEN: HUYAF4; ISSN: 1008-1011
PUBLISHER: Huaxue Yanjiu Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 143:305917
AB A group of α- and β-dialkylamino ketones were reduced enantioselectively by using BH3-THF and the in-situ formed chiral oxazaborolidine. The formed optically active aminoalc.-borane complexes, which, after deboration gave optically active amino alcs. with high enantiomeric excess. The effects of the substrate structure on the enantioselectivity of the reaction are also discussed.

L3 ANSWER 8 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:537764 CAPLUS
DOCUMENT NUMBER: 141:243031
TITLE: Highly Stereoselective Approach to Alk-2-yne-1,4-diols by Oxazaborolidine-Mediated Reduction of Alk-2-yne-1,4-diones
AUTHOR(S): Ariza, Xavier; Bach, Jordi; Berenguer, Ramon; Farras, Jaume; Fontes, Montserrat; Garcia, Jordi; Lopez, Marta; Ortiz, Jordi
CORPORATE SOURCE: Departament de Quimica Organica, Universitat de Barcelona, Barcelona, E-08028, Spain
SOURCE: Journal of Organic Chemistry (2004), 69(16), 5307-5313
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:243031
GI



I II

AB The authors performed borane-mediated reduction of a series of sym. alk-2-yne-1,4-diones, e.g. I, in the presence of a chiral oxazaborolidine to afford (R,R)-alk-2-yne-1,4-diols, e.g. II, in good yields and high stereoselectivities (up to 99.9% ee). In some cases, the stereochem. purity of II was improved by a two-step process: (i) temporary transformation of II into its vic-dibromo derivs. which allowed the removal of the minor meso isomer by chromatog., and (ii) regeneration of the enantioenriched diols II with SmI2. Reduction of the hexacarbonyldicobalt complexes derived from sym. alk-2-yne-1,4-diones, e.g. I, was also successful.
REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L3 ANSWER 9 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:560200 CAPLUS
DOCUMENT NUMBER: 139:260801
TITLE: Quantum Mechanical Study of Stereoselectivity in the Oxazaborolidine-Catalyzed Reduction of Acetophenone
AUTHOR(S): Alagona, Giuliano; Ghio, Caterina; Persico, Maurizio; Tomasi, Simone
CORPORATE SOURCE: Istituto per i Processi Chimico-Fisici, CNR, Pisa, I-56124, Italy
SOURCE: Journal of the American Chemical Society (2003), 125(33), 10027-10039
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Chiral oxazaborolidines, known as CBS catalysts after the work of Corey, Bakshi and Shibata, are used for the stereoselective reduction of prochiral ketones to secondary chiral alcs. Due to their relative low cost, ease of use, and high selectivity, their popularity has remarkably grown in the last 15 yr. Oxazaborolidine -catalyzed redns. have been much studied, both exptl. and computationally, by means of semiempirical methods. Though, a more accurate high level quantum mech. study on the complete system, capable of elucidating reliably the origins of stereoselectivity, is still lacking. Therefore, the acetophenone (PhMK) reduction with Corey's oxazaborolidine has been modeled for the first time with ab initio and DFT-B3LYP calcns. on the complete system as well as with AM1. Calcns. on the complexation of BH3 to CBS, which can occur only in a cis fashion with respect to the hydrogen on the stereogenic C-4 carbon atom, have allowed us to confirm the great rigidity of Corey's catalyst, possibly determining its excellent enantioselectivity. Acetophenone-CBS-BH3 complexes were characterized at various levels of theory, and it was found that the picture obtained depends heavily on the method adopted. A computational strategy for identifying the hydride transfer transition states of the competing pathways was developed and tested, using a model system for which the transition state geometry was already known. The application of the TS search method to the reduction of acetophenone allowed the characterization of the TS's for the competing pathways in this reaction, making it possible to predict with good quant. accuracy the stereochem. outcome of the reaction at all the levels of theory adopted. The characterization of the intermediate oxazadiboretane products confirmed that the highly exothermic hydride transfer provides the thermodynamical drive for the reaction.
REFERENCE COUNT: 78 THERE ARE 78 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L3 ANSWER 10 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:906244 CAPLUS
DOCUMENT NUMBER: 138:4202
TITLE: Preparation of iron-group metal-bound oxazaborolidines as reusable catalysts for enantioselective reduction of ketones
INVENTOR(S): Court, Jean; Lopez, Monique
PATENT ASSIGNEE(S): Centre National de la Recherche Scientifique CNRS, Fr.
SOURCE: PCT Int. Appl., 19 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

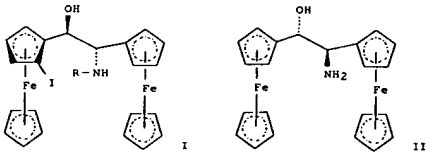
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002094837	A1	20021128	WO 2002-FR1602	20020513
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
FR 2824830	A1	20021122	FR 2001-6612	20010518
FR 2824830	B1	20030704		
AU 2002302721	A1	20021203	AU 2002-302721	20020513
EP 1387846	A1	20040211	EP 2002-730399	20020513
EP 1387846	B1	20060322		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
AT 321055	T	20060415	AT 2002-730399	20020513
US 2004133021	A1	20040708	US 2003-476668	20031104
US 6825370	B2	20041130		

PRIORITY APPLN. INFO.: FR 2001-6612 A 20010518
WO 2002-FR1602 W 20020513

OTHER SOURCE(S): CASREACT 138:4202; MARPAT 138:4202
AB The invention concerns oxazaborolidine compds. fixed on Raney Ni, Raney Co or Raney Fe, the method for preparing same, and the use of said compds. as reusable catalysts for enantioselective reduction of ketones to produce chiral alcs. For example, Raney Ni was treated in a suspension of THF with LiBH4 followed by BH3·(N,N-diethylaniline) or another borane adduct to give Ni5B. An amino alc. (e.g. (1S,2R)-(+)-2-amino-1,2-diphenylethanol) in THF was added to the Ni5B suspension to give the catalyst. Borane adduct is added to the catalyst and then the ketone in THF is reduced in its presence. P-fluoroacetophenone was reduced with 98% ee when the catalyst was used for the 1st time, followed by 91% and 90%, resp. for the 2nd and 3rd

L3 ANSWER 10 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
times. Product sepn. is easier using this system than when the catalysts are bound to org. polymers.
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 11 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:902346 CAPLUS
DOCUMENT NUMBER: 138:153636
TITLE: Asymmetric Synthesis of anti- and syn-β-Amino Alcohols by Reductive Cross-Coupling of Transition Metal-Coordinated Planar Chiral Arylaldehydes with Aldimines
AUTHOR(S): Tanaka, Yoshie; Taniguchi, Nobukazu; Kimura, Takayuki; Uemura, Motokazu
CORPORATE SOURCE: Department of Chemistry, Faculty of Integrated Arts and Sciences, Osaka Prefecture University, Osaka, 599-8531, Japan
SOURCE: Journal of Organic Chemistry (2002), 67(26), 9227-9237
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:153636
GI



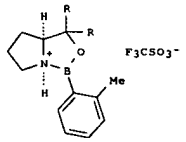
I II

AB SmI2-mediated cross-coupling of N-(tosyl)ferrocenylideneamine with planar chiral ferrocenecarboxaldehydes or benzaldehyde Cr tricarbonyl complexes gave diastereoselectively the corresponding anti-β-amino alc. derivs. in good yields, while N-(tosyl)benzylideneamine produced syn-β-amino alcs. by coupling with planar chiral arylaldehydes. E.g., SmI2 mediated reaction of (+)-(S)-α-iodoferrocenecarboxaldehyde with FcCH:NTs in THF (Fc = ferrocenyl) gave anti-β-amino alc. derivative I (R = p-MeC6H4SO2) in 94% yield with 94% ee while SmI2-mediated cross-coupling of PhCH:NTs with Cr(C6H6)(CO)3 gave syn-β-amino alc. PhCH(NHTs)CH(OAc)Ph with high diastereoselectivity (syn/anti = 97/3) in 73% overall yield after acetylation and subsequent demetalation. Dynamic kinetic resolution of a configurationally equilibrated reactive species generated from achiral N-(tosyl)ferrocenylideneamine and -benzylideneamine by reduction with SmI2 was observed in the cross-coupling with planar chiral arylaldehydes giving both antipodes of β-amino alcs. depending on the planar chirality. The obtained anti-β-amino alc. with the ferrocene ring was used as a chiral ligand for catalytic asym. reduction of acetophenone. E.g., catalytic asym. reduction of acetophenone in presence the oxazaborolidine formed in situ from anti-β-amino alc. II, MeB(OH)2, and B2H6 gave (S)-PhCH(OH)Me in 83% yield and 91% ee. A

L3 ANSWER 11 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
reaction mechanism was proposed to rationalize the obsd. stereoselectivity of the cross-coupling of N-(tosyl)ferrocenylideneamines with arylaldehydes. The efficient achievement of cross-coupling between ferrocenecarboxaldehyde and N-(arylsulfonyl)ferrocenylidenimines was attributed to different redn. potentials between both substrates.
REFERENCE COUNT: 94 THERE ARE 94 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 12 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:616524 CAPLUS
TITLE: Predictive modeling of chemical reactions
AUTHOR(S): Soltzberg, L. J.; Lee, Nancy E.; Honda, Ayako; Sanford, Michelle; Sekoni, Mojisola
CORPORATE SOURCE: Department of Chemistry, Simmons College, Boston, MA, 02115, USA
SOURCE: Abstracts of Papers, 224th ACS National Meeting, Boston, MA, United States, August 18-22, 2002 (2002), COMP-288. American Chemical Society: Washington, D. C.
CODEN: 69CZPZ
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB We have used off the shelf software (Spartan Pro) to model the outcomes of a variety of chemical reactions. Geometries of the reactant mols. are sep. optimized, and the mols. are given an initial orientation that might correspond to a reactive collision. Geometry optimization is then run on the assembly. Application of this procedure with a low level ab initio Hamiltonian has replicated the correct products and relative reactivities for the reduction of hydroquinone by various alkylammonia borane complexes. With a semi-empirical Hamiltonian, application of this method to the oxazaborolidine-catalyzed reduction of diverse ketones gives not only the correct products but reproduces the enantioselectivity of these redns. when carried out with a chiral catalyst.

L3 ANSWER 13 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:585820 CAPLUS
DOCUMENT NUMBER: 137:278751
TITLE: Broad-Spectrum Enantioselective Diels-Alder Catalysis by Chiral, Cationic Oxazaborolidines
AUTHOR(S): Ryu, Do Hyun; Lee, Thomas W.; Corey, E. J.
CORPORATE SOURCE: Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA
SOURCE: Journal of the American Chemical Society (2002), 124(34), 9992-9993
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:278751
GI



I

AB The cationic chiral Lewis acids I (R = Ph, 3,5-Me2C6H3), generated by triflic acid protonation of the corresponding neutral oxazaborolidines, serve as excellent catalysts for Diels-Alder addition of cyclopentadiene to a wide variety of dienophiles. Adducts have been obtained in excellent yield and enantioselectivity from α,β-unsatd. esters, lactones, and cyclic ketones. The absolute facial selectivity for each of these substrates follows a common pattern which differs from that observed with α,β-enals. The different reaction channels can be understood in terms of pathways via complexes (for α,β-enals) and (for α,β-enones and esters).
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 14 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:207077 CAPLUS
DOCUMENT NUMBER: 136:385883
TITLE: Asymmetric Diels-Alder Reactions Catalyzed by a Triflic Acid Activated Chiral Oxazaborolidine
AUTHOR(S): Corey, E. J.; Shibata, Takanori; Lee, Thomas W.
CORPORATE SOURCE: Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA
SOURCE: Journal of the American Chemical Society (2002), 124(15), 3808-3809
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:385883
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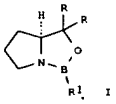

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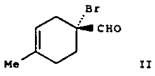

II

AB Oxazaborolidines I (R = 2-MeC6H4, 3,5-Me2C6H3; R1 = 2-MeC6H4), prepared from proline-derived α,α-diarylpyrrolidinemethanols and boroxines upon reflux in benzene, are activated by triflic acid to give powerful Lewis acid catalysts; in the presence of 6 mol% of the triflic acid-activated oxazaborolidines at -95°, the asym. Diels-Alder cycloaddns. of cyclic and acyclic dienes with either 2-Me or 2-bromoacrolein occur to give monocyclic or bicyclic cyclohexenecarboxaldehydes in 58-98% yields and in 91-97% ee. E.g., (S)-α,α-bis(3,5-dimethylphenyl)pyrrolidine-2-methanol was stirred in toluene with 1,3,5-tri(2-tolyl)boroxine and heated at 60° for 4 h followed by distillation to give I (R = 3,5-Me2C6H3; R1 = 2-MeC6H4) as a clear oil. E.g., 1.0 equivalent of triflic acid was added to a solution of I (R = 3,5-Me2C6H3; R1 = 2-MeC6H4) in methylene chloride; the solution was cooled to -95° and 2-bromoacrolein and 1,3-butadiene were added dropwise through a cannula; after stirring for 2 h at -95°, the mixture was warmed to room temperature and worked up to give cyclohexenecarboxaldehyde II in 98% yield and 97% ee. NMR studies of I (R = Ph; R1 = Me) in the presence of triflic acid showed that an equilibrium mixture of triflic acid-oxazaborolidine complexes exists; the species equilibrate slowly under the reaction conditions and more rapidly at 0°. The catalysts generated by treatment of I with triflic acid are estimated to be of similar acidity to triflic acid; catalysts generated from oxazaborolidines and methanesulfonic acid were ineffective at promoting Diels-Alder cycloaddn. reactions, allowing one to estimate the acid strength of the triflic acid complex of I. I were optimized for substitution at boron and at the α-position of the

L3 ANSWER 14 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
pyrrolidinemethanol moieties. The reactions are simple to conduct, reproducible, and economical, since only ca. 6 mol % of I is required; in addn., the chiral pyrrolidinemethanol precursors of I are readily recovered for reuse (>95% efficiency) and com. available. The reaction is effective with both cyclic and acyclic dienes. A mechanism accounting for the abs. and relative stereochem. of the Diels-Alder products is proposed.
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 15 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:877643 CAPLUS
DOCUMENT NUMBER: 136:278901
TITLE: Asymmetric reduction of amino ketones with borane and chiral oxazaborolidine catalyst
AUTHOR(S): Zhang, Ya-Wen; Shen, Zong-Xuan; Qin, Hong-Bing; Li, Yong-Hua; Yu, Kai-Bei
CORPORATE SOURCE: Department of Chemistry and Chemical Engineering, Suzhou University, Suzhou, 215006, Peop. Rep. China
SOURCE: Chinese Journal of Chemistry (2001), 19(11), 1130-1135
CODEN: CJOCEV; ISSN: 1001-604X
PUBLISHER: Science Press
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:278901

AB Some α-(dialkylamino) ketones and β-(dialkyl amino) ketones were reduced stereoselectively by 2 mol of borane-tetrahydrofuran in the presence of 10 mol% of an in situ-formed chiral oxazaborolidine, followed by diluted hydrochloric acid. The catalysts in this study included (3aR)-tetrahydro-1-methyl-3,3-diphenyl-1H,3H-pyrrolo[1,2-c][1,3,2]oxazaborole, (3aS)-tetrahydro-1-methyl-3,3-diphenyl-1H,3H-pyrrolo[1,2-c][1,3,2]oxazaborole and (4R,5S)-2-methyl-4,5-diphenyl-1,3,2-oxazaborolidine. The resulting amino alc.-borane complexes were treated with hydrogen chloride-glycol-methanol to give the optically active amino alc. with the ee up to 99%. For example, the reduction of 3-(4-morpholinyl)-1-phenyl-1-propanone gave (+)-(αR)-α-phenyl-4-morpholinepropanol in 87.3% yield. The intermediate α-phenyl-4-morpholinepropanol-borane complex was characterized by x-ray crystallog.

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 16 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:536261 CAPLUS
DOCUMENT NUMBER: 134:147384
TITLE: An efficient synthesis of (1S, 2R)-1-amino-2-indanol, a key intermediate of HIV protease inhibitor, indinavir
AUTHOR(S): Demir, Ayhan S.; Aksoy-Cam, Hilal; Camkerten, Nurettin; Hamamci, Haluk; Doganel, Fatos
CORPORATE SOURCE: Department of Chemistry, Middle East Technical University, Ankara, 06531, Turk.
SOURCE: Turkish Journal of Chemistry (2000), 24(2), 141-146
CODEN: TJCHE3; ISSN: 1300-0527
PUBLISHER: Scientific and Technical Research Council of Turkey
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:147384

AB (1S,2R)-1-amino-2-indanol, a key component of HIV protease inhibitor was prepared in four steps starting from indanone. The Mn(OAc)3 mediated acetoxylation of indanone followed by fungus catalyzed hydrolysis of acetoxyindanone furnished optically pure α-hydroxyindanone. Formation and enantioselective reduction of oxime ether of 2-hydroxyindanone afforded (1S,2R)-1-amino-2-indanol in 97% cis selectivity.

REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 17 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:188699 CAPLUS
DOCUMENT NUMBER: 133:89130
TITLE: Nondynamic Kinetic Resolution of Configurationally Stable Biaryl Lactones by Reduction with Oxazaborolidine-Activated Borane: AM1 Studies and Experimental Verification
AUTHOR(S): Bringmann, Gerhard; Hinrichs, Juergen; Kraus, Juergen; Wuzik, Andreas; Schulz, Tanja
CORPORATE SOURCE: Institut fuer Organische Chemie, Universitaet Wuerzburg, Wuerzburg, D-97074, Germany
SOURCE: Journal of Organic Chemistry (2000), 65(8), 2517-2527
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:89130
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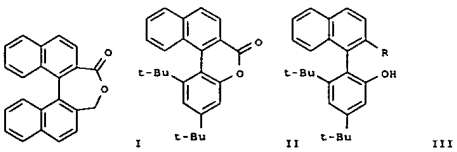

I II III

AB The complete mechanistic course of the atroposelective ring opening of a lactone-bridged biaryl, dinaphth[2,1-c:1',2'-e]oxepin-3-(5H)-one (3 = I), with a chiral oxazaborolidine-BH3 complex was calculated using the semiempirical AM1 method. The first hydride transfer to the activated carbonyl function of the adduct complexes was elaborated to be the selectivity-determining step in the postulated five-step mechanism. The calculated enantioselectivity is in good accordance with the exptl. results, so that related calcns. were performed on the atroposelective ring opening of a sterically strongly hindered and therefore also configurationally stable six-membered biaryl lactone, 1,3-di-tert-butyl-6H-benzo[b]naphtho[1,2-d]pyran-6-one (6f = II). These calcns. predicted a highly (M)-selective reduction of 6f (kM/kP = 358 at -78 °C), which, after the smooth preparation of 6f by intramol. biaryl coupling in high yields, was fully confirmed exptl. (kM/kP > 200 at -78 °C). Isolation of the intermediate hydroxy aldehyde (M)-14 [(M)-III, R = CHO] at the beginning of the reaction with the same enantiomeric excess as found for the corresponding alc. (M)-7f [(M)-III, R = CH2OH] conclusively showed the first hydride transfer step to determine the selectivity of this process. The good agreement of computationally predicted and exptl. confirmed values proves the suitability of the AM1 method for mechanistic studies on even such complex reactions and opens a most efficient overall synthesis of sterically highly hindered biaryls, in excellent chem. (for the ring closure) and optical (for the ring cleavage) yields and for any desired axial configuration.

REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 18 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:467746 CAPLUS
DOCUMENT NUMBER: 131:310376
TITLE: Catalytic enantioselective reactions. Part 16. Oxazaborolidine-catalyzed asymmetric borane reduction of α-keto acetals
AUTHOR(S): Cho, Byung Tae; Chun, Yu Sung
CORPORATE SOURCE: Chunchon, Department of Chemistry, Hallym University, Kangwon Do, 200-702, S. Korea
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1999), (15), 2095-2100
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:310376
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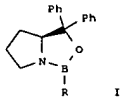

I

AB Asym. redns. of α-keto acetals, e.g., PhCOCH(OEt)2, using various oxazaborolidines, e.g., I (R = H, Me, Bu, Ph), and borane reagents, e.g., BH3·THF, PhNEt2·BH3, as catalysts and hydride sources, resp., were compared. The reduction catalyzed by reagents I (R = H, Me) with N-phenylamine-borane reagents provided chiral α-hydroxy acetals, e.g., (S)-PhCH(OH)CH(OEt)2, with very high enantioselectivities for most aromatic analogs.
REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 19 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:338202 CAPLUS
DOCUMENT NUMBER: 127:50692
TITLE: Chiral intramolecular amine-borane complexes as reducing agents for prochiral ketones
AUTHOR(S): Toumelin, Jean-Brice Le; Baboulene, Michel
CORPORATE SOURCE: Laboratoire des IMRCP, UMR 5623 (CNRS), Universite P. Sabatier, Toulouse, 31062, Fr.
SOURCE: Tetrahedron: Asymmetry (1997), 8(8), 1259-1265
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:50692
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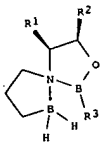

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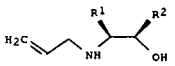

II

AB A new family of chiral amine-borane complexes, the N-spiroazaborolidines I, were synthesized from reaction of allylaminoethanol II (e.g., R1 = H, Me, R2 = Me, Ph) with R3B(OH)2 (R3 = Me, Ph, H) followed by cyclization with borane dimethylsulfide. I are stable, convenient to use, and are excellent reducing agents of prochiral ketones (yieldreduction ≥ 95%). However, poor enantioselectivity was obtained (ee ≤ 38%). The configuration of these mols. (cis position between Baza and the substituent on the Boxaza), unfavorable for a good approach of the ketone, is a possible explanation. These results show the importance of the stereochem. of the N atom in amine-borane complexes for asym. synthesis.
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 20 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:705586 CAPLUS
DOCUMENT NUMBER: 126:8173
TITLE: Highly Enantioenriched Propargylic Alcohols by Oxazaborolidine-Mediated Reduction of Acetylenic Ketones
AUTHOR(S): Bach, Jordi; Berenguer, Ramon; Garcia, Jordi; Loscertales, Teresa; Vilarrasa, Jaume
CORPORATE SOURCE: Departament de Quimica Organica, Universitat de Barcelona, Barcelona, 08028, Spain
SOURCE: Journal of Organic Chemistry (1996), 61(25), 9021-9025
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:8173
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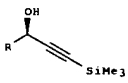

I

II

AB An efficient and general approach to highly enantiomerically enriched propargylic alcs., e.g., I (R = PhCH2CH2), by borane-mediated, oxazaborolidine, e.g., II, catalyzed reduction of ketones, e.g., PhCH2CH2COCH.tplbond.CSiMe3, is described.
REFERENCE COUNT: 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 21 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:655858 CAPLUS
DOCUMENT NUMBER: 121:255858
TITLE: A combined synthetic and ab initio study of chiral oxazaborolidines structure and enantioselectivity relationships
AUTHOR(S): Quallich, George J.; Blake, James F.; Woodall, Teresa M.
CORPORATE SOURCE: Central Research Division, Pfizer Inc., Groton, CT, 06340, USA
SOURCE: Journal of the American Chemical Society (1994), 116(19), 8516-25
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:255858
AB Investigations into the relationship of oxazaborolidine structure to the enantioselectivity obtained in the reduction of prochiral ketones revealed the intrinsic power of the mol. recognition element in the catalytic reduction This mol. recognition, two-point binding of borane and the ketonic oxygen atom by the oxazaborolidine, assembles a trimol. complex which provides high enantiomeric excess. Enantiomeric excess was demonstrated to be dependent on the extent to which one oxazaborolidine face was precluded from attaining two-point binding and on nonbonded interactions that developed during formation of the borane-oxazaborolidine complex. As a result, erythro-substituted oxazaborolidines were demonstrated to be useful catalysts for enantioselective reduction of prochiral ketones. Ab initio MO calcns. have been used to locate possible complexes and transition state assemblies that correspond to catalyst-borane and the trimol. complex on a proposed reduction pathway. Geometry optimizations were carried out at the 3-21G, 6-31G(d), and MP2/6-31G(d) levels of theory. Correlation energies were computed via Moeller-Plesset perturbation theory to the second order (MP2). Relative activation energies establish correctly the observed enantioselectivity of the two best oxazaborolidine catalysts in this study. Addnl., the diminished enantioselectivity of N-methyl-substituted catalysts was traced to conformational changes in the exo transition state. Though the relative energies obtained from the various levels of theory are similar, absolute complexation and activation energies are found to vary considerably with the level of theory employed. The existence of key intermediates was found to depend on the level of theory.

L3 ANSWER 22 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:508893 CAPLUS
DOCUMENT NUMBER: 121:108893
TITLE: Quantum chemical modeling of chiral catalysis. Part 18. Conformational studies on chiral N-sulfonylated 1,3,2-oxazaborolidines and related aldehyde complexes potentially involved in the catalytic asymmetric Diels-Alder reactions
AUTHOR(S): Nevalainen, Vesa
CORPORATE SOURCE: Div. Org. Chem., Univ. Helsinki, Helsinki, SF-00014, Finland
SOURCE: Tetrahedron: Asymmetry (1994), 5(4), 767-72
CODEN: TASYE3; ISSN: 0957-4166
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

I

AB Properties of Lewis acidic oxazaborolidines were investigated by means of ab initio MO methods [RHF, N-sulfonylated 1,3,2-oxazaborolidine (I) as a model]. Energies of the coordination of aldehydes to oxaazaborolidines were estimated by using formaldehyde and acrolein adducts of I as models. Energies (MP2/6-31G//6-31G) of the coordination of formaldehyde to I were determined The corresponding energies of the formation of acrolein adducts , were higher.

L3 ANSWER 23 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:482602 CAPLUS
DOCUMENT NUMBER: 121:82602
TITLE: Convenient procedures for the asymmetric reductions utilizing α,α-diphenylpyrrolidinemethanol and borane complexes generated using the I2/NaBH4 system
AUTHOR(S): Periasamy, Mariappan; Kanth, J. V. Bhaskar; Prasad, A. S. Bhanu
CORPORATE SOURCE: Sch. Chem., Univ. Hyderabad, Hyderabad, 500 134, India
SOURCE: Tetrahedron (1994), 50(21), 6411-16
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:82602
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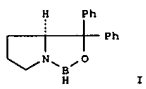

I

AB Prepns. of oxazaborolidine in situ in benzene using α,α-di-phenylpyrrolidinemethanol and diborane, generated from the I-Na borohydride system are described. The oxazaborolidine (10 mol %), generated by the reaction of α,α-diphenylpyrrolidinemethanol and diborane in benzene followed by heating with N,N-diethylaniline, in combination with borane-THF complex reduces acetophenone to 1-phenylethanol in 94.7% ee. Formation of the oxazaborolidine complex I was facilitated in the presence of an amine.

L3 ANSWER 24 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:409461 CAPLUS
DOCUMENT NUMBER: 121:9461
TITLE: Quantum-chemical modeling of chiral catalysis. Part 15. On the role of hydride-bridged borane-alkoxyborane complexes in the catalytic enantioselective reduction of ketones promoted by chiral oxazaborolidines
AUTHOR(S): Nevalainen, Vesa
CORPORATE SOURCE: Div. Org. Chem., Univ. Helsinki, Helsinki, SF-00014, Finland
SOURCE: Tetrahedron: Asymmetry (1994), 5(2), 289-96
CODEN: TASYE3; ISSN: 0957-4166
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Hydride-bridged borane-alkoxyborane complexes of oxazaborolidines were investigated by means of ab initio MO methods (RHF). The complexes were found to be stable in the absence of Lewis basic solvents. In the presence of a Lewis basic solvent the borane-alkoxyborane complexes were predicted to decompose leading to the formation of borane-solvent complexes of the oxazaborolidines. A new class of oxazaborolidine catalysts, of which the mechanism of regeneration would be based on borane-borane hydride exchange, was invented.

L3 ANSWER 25 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:217770 CAPLUS
DOCUMENT NUMBER: 120:217770
TITLE: Quantum chemical modeling of chiral catalysis. Part 13. Role of borane O-adducts in the enantioselective reduction of ketones catalyzed by chiral oxazaborolidines
AUTHOR(S): Nevalainen, Vesa
CORPORATE SOURCE: Div. Org. Chem., Univ. Helsinki, Helsinki, 00014, Finland
SOURCE: Tetrahedron: Asymmetry (1993), 4(9), 2001-10
CODEN: TASYE3; ISSN: 0957-4166
DOCUMENT TYPE: Journal
LANGUAGE: English
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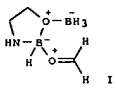

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AB Plausible reactions of Lewis bases (ketones and ethers) with borane O-adducts of chiral oxazaborolidines, e.g., I, used as catalysts in the enantioselective reduction of ketones were investigated by means of ab initio MO methods. Properties of the O-adducts were found to be different from those of the corresponding N-adducts. The O-adducts were not able to form complexes with ketones and ethers similar to those of the corresponding N-adducts proposed to be essential for the performance of oxazaborolidines as chiral catalysts in the enantioselective reduction of ketones.

L3 ANSWER 26 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:670371 CAPLUS
DOCUMENT NUMBER: 119:270371
TITLE: Quantum chemical modeling of chiral catalysis. Part 12. Influence of the nature of the ring system on binding in ketone-borane complexes of chiral oxazaborolidines used as catalysts in the enantioselective reduction of ketones
AUTHOR(S): Nevalainen, Vesa
CORPORATE SOURCE: Div. Org. Chem., Univ. Helsinki, SF-00014, Finland
SOURCE: Tetrahedron: Asymmetry (1993), 4(7), 1597-602
CODEN: TASYE3; ISSN: 0957-4166
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Coordination of ketones (formaldehyde as a model) to borane N-adducts of 1-aza-2-bora-3-oxabicyclo[3.3.0]octane (I) and 1,3,2-oxazaborolidine was investigated by means of ab initio MO methods. Coordination energies were more pos. in the case of the more strained and rigid bicyclic I. Why I derivs. can perform better as catalysts than the corresponding simple 1,3,2-oxazaborolidines is discussed.

L3 ANSWER 27 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:670321 CAPLUS
DOCUMENT NUMBER: 119:270321
TITLE: Quantum chemical modeling of chiral catalysis. Part 10. Complexes of carbonyl compounds with chiral N-sulfonylated 1,3,2-oxazaborolidines used as catalysts in the enantioselective Diels-Alder reactions
AUTHOR(S): Nevalainen, Vesa
CORPORATE SOURCE: Div. Org. Chem., Univ. Helsinki, SF-00014, Finland
SOURCE: Tetrahedron: Asymmetry (1993), 4(7), 1565-8
CODEN: TASYE3; ISSN: 0957-4166
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Formation of complexes of carbonyl compds. with N-sulfonylated 1,3,2-oxazaborolidines was investigated by means of ab initio MO methods. An unusual mode of coordination leading to the formation of a six-membered ring (boat conformation) was observed as formaldehyde was used as a model of carbonyl compds. and an adduct of formaldehyde to N-sulfonyl-1,3,2-oxazaborolidine as a model of the complexes. In this six-ring system, the oxygen of formaldehyde was bound to the boron of oxazaborolidine and the carbon to one of the oxygens of the N-sulfonyl group. As a consequence of this unusual complexation, the C:O double bond of formaldehyde lengthened substantially; the planar shape of the carbonyl was distorted and the pos. charge of the carbonyl carbon increased about 100%.

L3 ANSWER 28 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:234104 CAPLUS
DOCUMENT NUMBER: 118:234104
TITLE: Quantum chemical modeling of chiral catalysis. Part 8. The conformational freedom of the ketone of ketone-borane complexes of oxazaborolidines used as catalysts in the enantioselective reduction of ketones
AUTHOR(S): Nevalainen, Vesa
CORPORATE SOURCE: Dep. Chem., Univ. Helsinki, Helsinki, SF-00100, Finland
SOURCE: Tetrahedron: Asymmetry (1992), 3(12), 1563-72
CODEN: TASYE3; ISSN: 0957-4166
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Standard ab initio MO methods were employed to study conformational freedom of the ketone of ketone-borane complexes of chiral oxazaborolidines used as catalysts for the enantioselective reduction of ketones. A formaldehyde-borane complex of 1,3,2-oxazaborolidine was used as a model system. A new conformation was found which was energetically more advantageous than the original one predicted by Corey et al. The new conformation was predicted to be destabilized by bulky substituents at the C-5 of the ring. A new class of potential oxazaborolidine catalysts for the enantioselective reduction of ketones was found.

L3 ANSWER 29 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:425621 CAPLUS
DOCUMENT NUMBER: 117:25621
TITLE: Quantum chemical modeling of chiral catalysis. Part 4. On the hydride transfer in ketone complexes of borane adducts of oxazaborolidines and regeneration of the catalyst
AUTHOR(S): Nevalainen, Vesa
CORPORATE SOURCE: Dep. Chem., Univ. Helsinki, Helsinki, SF-00100, Finland
SOURCE: Tetrahedron: Asymmetry (1991), 2(11), 1133-55
CODEN: TASYE3; ISSN: 0957-4166
DOCUMENT TYPE: Journal
LANGUAGE: English
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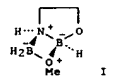

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AB Hydride transfer and regeneration steps in ketone complexes of borane-oxazaborolidine adducts functioning as chiral catalysts were investigated by using ab initio MO methods. The hydride transfer was found to be highly exothermic. Formation of a novel 1,3-oxazadiboretane structure (e.g., I) was found to precede the regeneration of the catalyst. The regeneration occurring via a cleavage of the 1,3-oxazadiboretane ring was found to require about 10% of the energy released in the hydride transfer. Reactions being potentially involved in the deactivation of oxazaborolidine catalysts were found.

L3 ANSWER 30 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:655308 CAPLUS
DOCUMENT NUMBER: 115:255308
TITLE: Quantum chemical modeling of chiral catalysis. Part 3. On the role of a Lewis basic solvent in the mechanism of catalytic enantioselective reduction of carbonyl compounds by chiral oxazaborolidinea
AUTHOR(S): Nevalainen, Vesa
CORPORATE SOURCE: Dep. Chem., Univ. Helsinki, Helsinki, SF-00100, Finland
SOURCE: Tetrahedron: Asymmetry (1991), 2(8), 827-42
CODEN: TASYE3; ISSN: 0957-4166
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Structures and energies of formation of complexes of Lewis basic solvents with borane-oxazaborolidine adducts functioning as chiral catalysts were investigated by using ab initio MO methods (6-31G*//6-31G*). Formation of complexes of water with a borane adduct of 1,3,2-oxazaborolidine and simpler analogs of it was examined as a model system. Coordination of water to the borane adduct of 1,3,2-oxazaborolidine stabilized the adduct by about 50-60% of that of a free borane. Substitution of water bound to the borane adduct of the catalyst by formaldehyde required about 4-5 times more energy than coordination of formaldehyde to the corresponding solvent-free borane adduct.

L3 ANSWER 31 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:583405 CAPLUS
DOCUMENT NUMBER: 115:183405
TITLE: Quantum chemical modeling of chiral catalysis. Part 2. On the origin of enantioselection in the coordination of carbonyl compounds to borane adducts of chiral oxazaborolidines
AUTHOR(S): Nevalainen, Vesa
CORPORATE SOURCE: Dep. Chem., Univ. Helsinki, Helsinki, SF-00100, Finland
SOURCE: Tetrahedron: Asymmetry (1991), 2(6), 429-35
CODEN: TASYE3; ISSN: 0957-4166
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Energies of formation and structural parameters of HCHO and MeCHO complexes of a model system of borane adducts of oxazaborolidine type of chiral reduction catalysts (CBS reduction) were calculated by using ab initio MO methods (6-31G*//6-31G*). The energetic preference was determined for the formation of complexes in which the Lewis acidic boron of the borane adduct of an oxazaborolidine would coordinate either syn or anti to the Me group of acetaldehyde. The formation of anti complex was favored by 15.2 kJ mol-1 which corresponds to a relative anti:syn abundance ratio of 461:1 and an enantiomeric excess of 99.8%.

L3 ANSWER 32 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:429427 CAPLUS
DOCUMENT NUMBER: 115:29427
TITLE: Quantum chemical modeling of chiral catalysis. On the mechanism of catalytic enantioselective reduction of carbonyl compounds by chiral oxazaborolidines
AUTHOR(S): Nevalainen, Vesa
CORPORATE SOURCE: Dep. Chem., Univ. Helsinki, Helsinki, SF-00100, Finland
SOURCE: Tetrahedron: Asymmetry (1991), 2(1), 63-74
CODEN: TASYE3; ISSN: 0957-4166
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Energies of formation and structural parameters of two model systems of oxazaborolidine type of chiral reduction catalysts (CBS reduction), their borane adducts, and formaldehyde complexes of the borane adducts were calculated by using ab initio MO methods. Energies of the formation of formaldehyde complexes in which the borane and carbonyl were cis about the B-N bond of the oxazaborolidine ring were found to be slightly pos. The corresponding trans coordination was found to be repulsive. A new class of potential chiral catalysts which also contain the substructure O-B-N was found.

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